

# Perfluorovaleric acid

2706-90-3 | DTXSID6062599

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1.75

Global applicability domain: Outside

Local applicability domain index: 4.37e-01

Confidence level: 5.46e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Sulfone, methyl pentafluorophenyl</div> <div>Measured: 1.46</div> <div>Predicted: 2.02</div>	<div>Image not found</div> <div>Benzoic acid, 3,6-dichloro-2-hydroxy-</div> <div>Measured: 2.30</div> <div>Predicted: 1.70</div>	<div>Image not found</div> <div>Dicamba</div> <div>Measured: 1.50</div> <div>Predicted: 1.95</div>
<div>Image not found</div> <div>Chlorfenac</div> <div>Measured: 1.80</div> <div>Predicted: 1.86</div>	<div>Image not found</div> <div>2,3,6-Trichlorophenylacetic acid sodium salt</div> <div>Measured: 1.72</div> <div>Predicted: 1.86</div>	